ALCF Early Science Program

ESP Kick-Off Workshop
Project Plan Presentation

Petascale Simulations of Turbulent Nuclear Combustion

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Project Overview

- **Science Objective:**
  - Type Ia (thermonuclear-powered) supernovae are important in understanding the origin of the elements and a critical tool in cosmology
  - The Flash Center will carry out large-scale, 3D simulations of two key physical processes in Type Ia supernovae that are not fully understood
  - These simulations will reduce the uncertainties in simulating Type Ia supernova explosions much more accurately, and so understand them much better

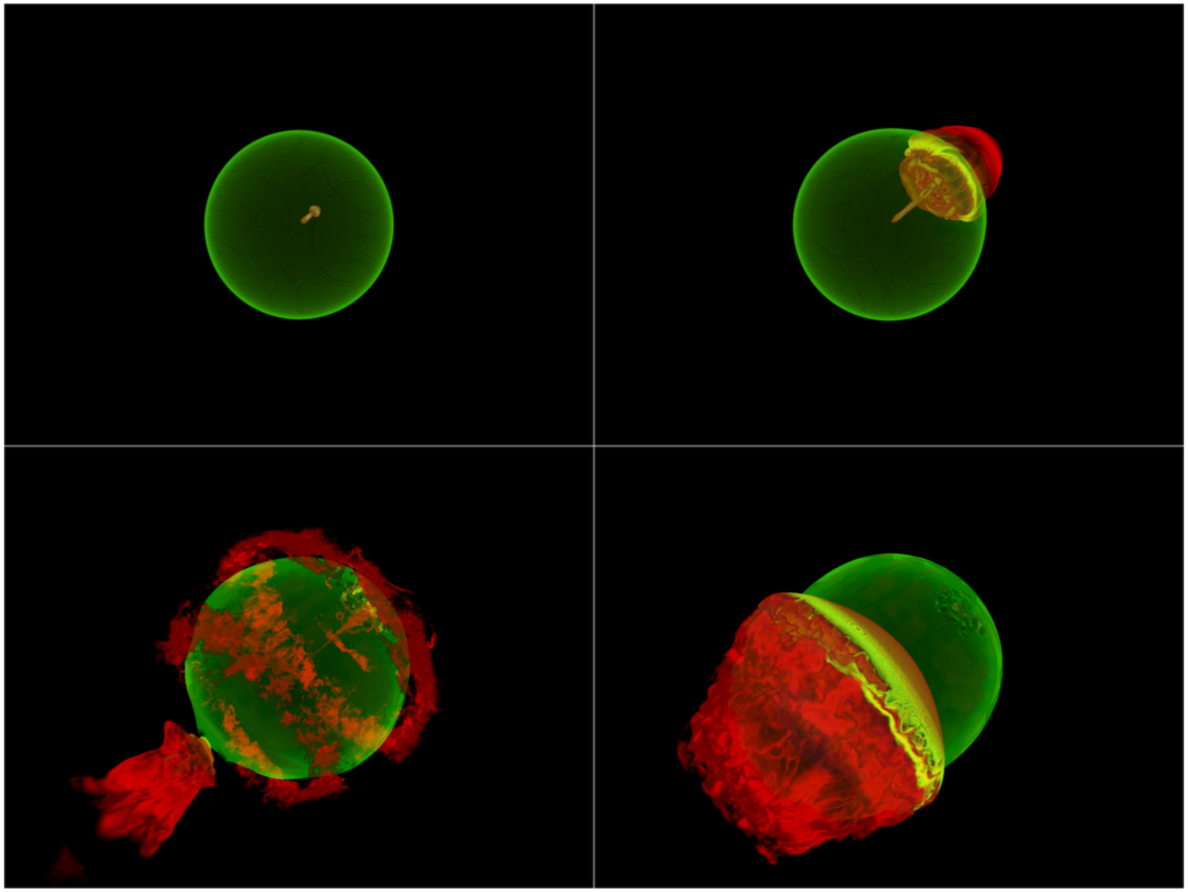
Scientific Field: Astrophysics

Codes: FLASH

Key Physical Processes in Type Ia Supernovae That Are Not Fully Understood

- **Buoyancy-driven turbulent nuclear combustion**
  - Determines the amount of nuclear energy released during the ordinary flame burning phase (the so-called ``deflagration phase") of the explosion, which lasts ~ 1 second
  - Amount of nuclear energy released during this phase determines the amount that the white dwarf star expands before it detonates, which determines how luminous the Type Ia supernova is
- **Transition from nuclear burning in the flamelet regime to distributed nuclear burning**
  - Observations show a detonation occurs that incinerates the star and releases most of the nuclear energy that powers the explosion
  - Transition is thought to set the stage for initiation of a detonation wave in some Type Ia supernova models
- **Neither physical process is fully understood**

Discovery of Entirely New Mechanism for SN Ia: Gravitationally Confined Detonation



Calder et al. (2003); Plewa, Calder and Lamb (2004); Townsley et al. (2007); Jordan et al. (2008); Meakin et al. (2009)

The Center for Astrophysical Thermonuclear Flashes

Simulation of the Deflagration and Detonation Phases of a Type Ia Supernovae

30 initial bubbles in 100 km radius.
Ignition occurs 80 km from the center of the star.
Hot material is shown in color and stellar surface in green.

This work was supported in part at the University of Chicago by the DOE NNSA ASC ASAP and by the NSF. This work also used computational resources at LBNL NERSC awarded under the INCITE program, which is supported by the DOE Office of Science.

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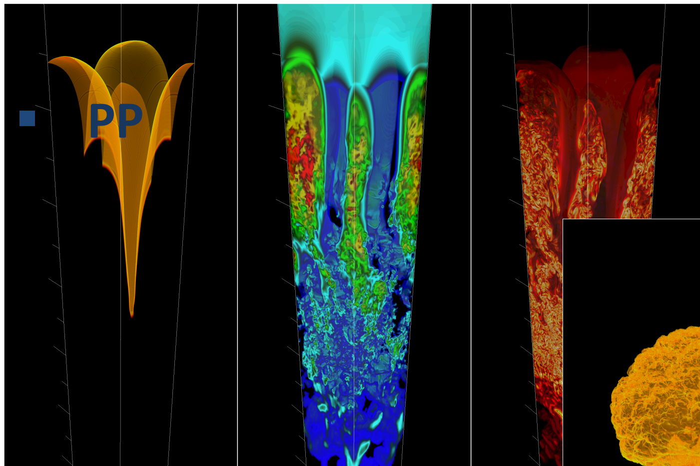
Mira Simulation Strategy

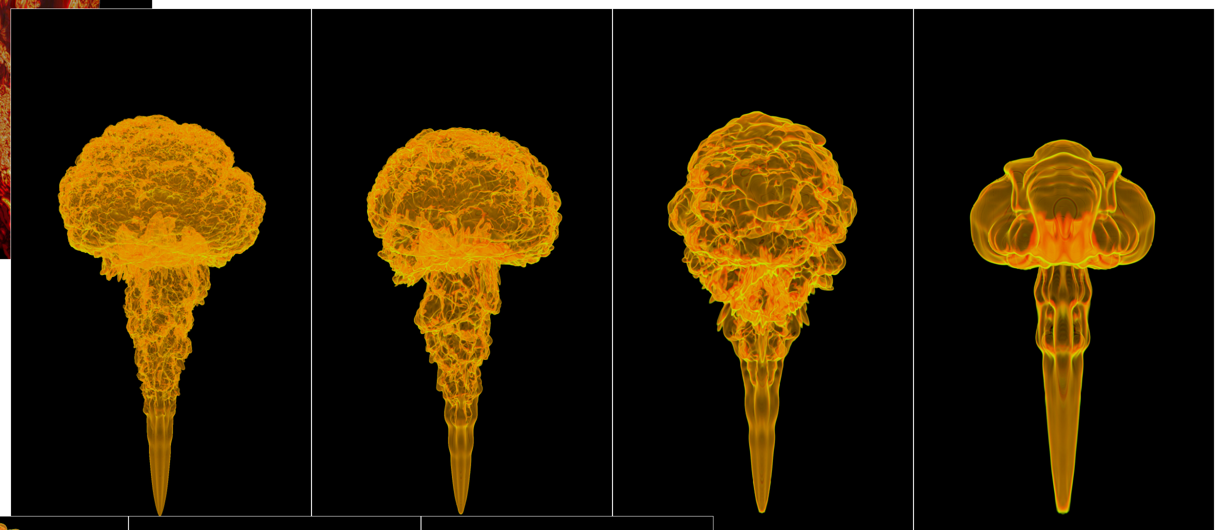
- **In studying buoyancy-driven turbulent nuclear burning, we will carry out large-scale, 3D simulations for three different physical situations:**
  - An initially planar flame in a rectilinear domain at constant acceleration of gravity *g* and nearly constant density ρ
  - A flame bubble in a rectilinear domain at constant *g* and nearly constant ρ
  - A flame bubble in a white dwarf star, in which case both *g* and ρ vary with distance from the center of the star
- **Mira will enable us to do simulations with > 20 times more grid points**
- **Specific goal of simulations is to determine the length scale that governs the rate of nuclear burning, which will enable us to develop an accurate sub-grid model of this key physical process**

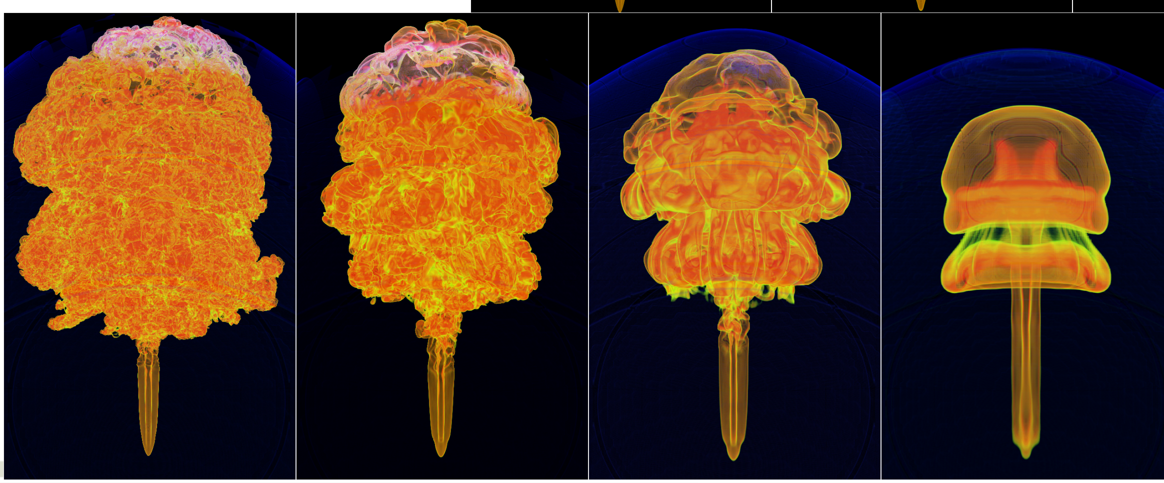
3D Verification Simulations of Buoyancy-Driven Turbulent Nuclear Combustion



Initially Planar Flame
In Rectilinear Domain
at Constant g and ρ

Flame Bubble in Rectilinear
Domain at Constant g and ρ





Flame Bubble
in White Dwarf Star

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Simulation of Buoyancy-Driven Turbulent Nuclear Burning for a Froude Number of 0.010

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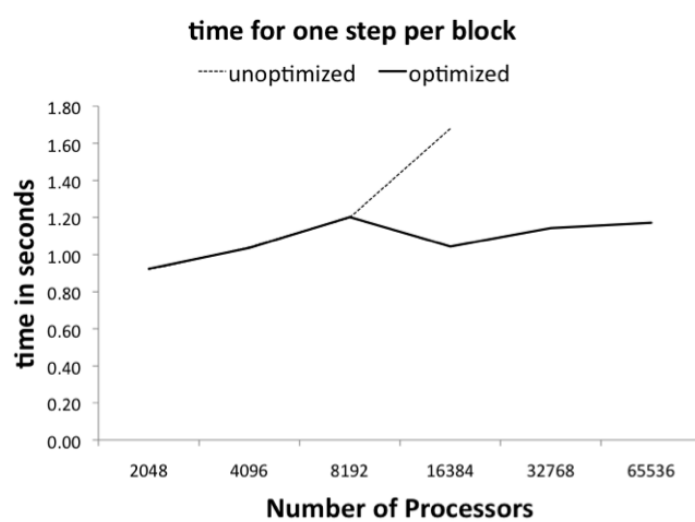
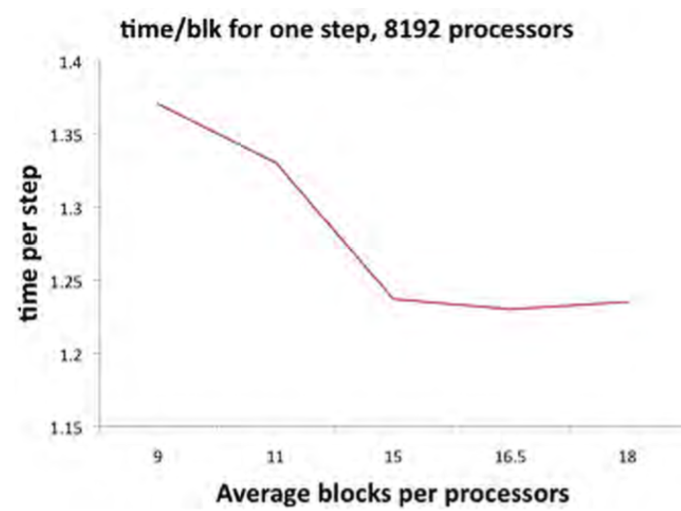
Computational Approach, Numerical Methods

- **Multi-scale Eulerian compressible hydrodynamics**
  - Piecewise parabolic method (PPM)
    - Generalized equation of state
      - Applies to ionized plasma of arbitrary degeneracy
- **Dynamic adaptive mesh refinement (AMR)**
  - PARAMESH: block structure octtree
- **Advection-diffusion-reaction flame model**
- **Constant gravity**

Parallelism and Existing Implementation

- **Partition mesh(and particles) among MPI processes**
  - Communication required when:
    - Exchanging subdomain boundary data
    - Mapping to and from finer blocks
    - Mesh load rebalanced
    - Particles move between subdomains
    - Solvers such as multipole, multigrid and FFT
- **MPI everywhere (no threads)**
- **Current Performance/Scalability**





Library and Tool Dependencies

- **Libraries**
  - MPI
  - HDF5 (parallel) or pNetCDF (parallel I/O)
  - PARAMESH (included with distribution)
  - Chombo (AMR and associated solvers *(planned)*)
- **Tools**
  - IDL or VisIt (visualization)

Anticipated Modifications for Blue Gene/Q

- **Implement node-level parallelism: threads**
  - FLASH already divides grids into blocks
  - Multiple blocks assignable per MPI process
  - Exploit this to process blocks concurrently on threads
    - One MPI process per Mira node
    - 200-250 blocks per node
      - Distribute among threads/cores

- **Add Chombo library to FLASH**
  - Patch-based AMR more suitable for some applications
  - Chombo has roadmap to petascale and exascale

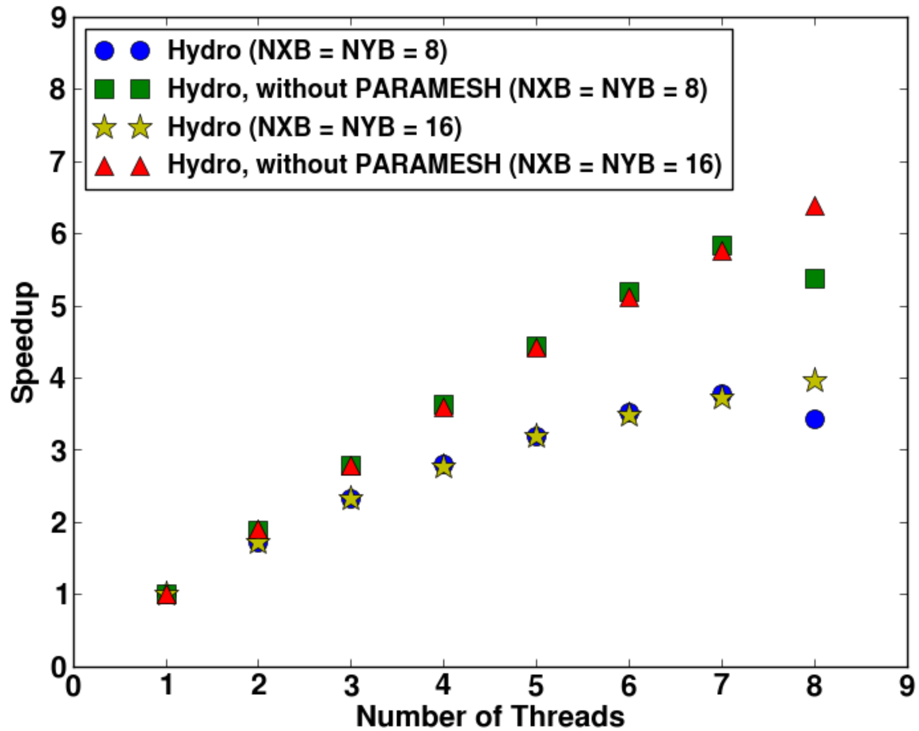
- **Performance and scaling needed to run proposed problem on Mira:**
  - 20x gridpoints of present-day simulations
    - 20x gridpoints within inertial range in today's Roadrunner turbulence simulations

Plan for Next 6 Months Effort

- **Help find and hire a project postdoc**
- **Continue collaborative research into parallel I/O performance of the code with ANL**
- **Introduce threads in main code kernels:**
  - Experimentation in progress (results in next slide)
  - Transition to code
- **Finish enabling use of Chombo**
- **Benchmark performance on BG/P w.r.t.:**
  - Threads at block level
  - Threads at sub-block level
  - Incorporation of parallel I/O research
- **Use projections to estimate performance on BG/Q**

Block and Sub-block Threading Experiments

Block level threading (Hydro)



Sub-block level threading (EOS)